

# Canonically invariant formulation of Langevin and Fokker-Planck equations

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We present a canonically invariant form for the generalized Langevin and Fokker-Planck equations. We discuss the role of constants of motion, and the construction of conservative stochastic processes.

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Consider the usual Langevin equation:

$$m\ddot{q}_i = -\frac{\partial V}{\partial q_i} - \dot{q}_i + \xi_i(t) \quad (1)$$

with  $\xi_i(t)$  Gaussian white noises  $\langle \xi_i(t)\xi_j(t') \rangle = 2T\delta_{ij}\delta(t-t')$ , and  $T$  the temperature of the thermic bath. Rewriting this as a set of phase-space equations:

$$\begin{cases} \dot{q}_i = \frac{p_i}{m} \\ \dot{p}_i = -\frac{\partial V}{\partial q_i} - \frac{p_i}{m} + \xi_i(t) \end{cases} \quad (2)$$

we notice two things. First, the form of the first equation is restricted to a hamiltonian  $H$  of the form  $H = \sum_i p_i^2/m + V(q)$ . Second, the interaction with the bath has introduced an assymetry in the treatment of coordinates and momenta. We shall in what follows formulate the Langevin and Fokker-Planck processes in a way that treats all phase-space variables on an equal footing.

In general, Langevin equations can be motivated [1] [2] by considering the system with Hamiltonian  $H$ , coupled to an infinite set of harmonic oscillators with random phases at some initial time and energies given by equipartition at temperature  $T$ . Upon solving for the oscillators, and reinjecting their dependence on the equation of motion, one gets a Langevin equation which can be made Markovian by a suitable choice of distribution of the oscillators' frequencies.

Actually, (1,2) are associated with a particular coupling of the form:

$$H_{coup} = \sum_i q_i \left[ \sum_{a=1}^N A_a^i y_a^i \right] \quad (3)$$

where  $y_a^i$  are the coordinates of the oscillators of frequencies  $\omega_a^i$ .

In order to obtain a canonically invariant generalization, one can repeat the exercise with a coupling with the 'bath' of oscillators of a more general form:

$$H_{coup} = \sum_i \sum_{a=1}^N [A_a^i G_a^1(\mathbf{q}, \mathbf{p}) y_a^i + B_a^i G_a^2(\mathbf{q}, \mathbf{p}) \dot{y}_a^i] \quad (4)$$

Performing the usual steps, one arrives at the following Langevin equation, valid for any phase-space variable  $A(\mathbf{q}, \mathbf{p})$ , in particular the coordinates and momenta  $q_i, p_i$ :

$$\dot{A} = \kappa\{A, H\} + \sum_j \{A, G_j\}(\xi_j(t) + \{G_j, H\}) \quad (5)$$

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We have explicitated an inverse time-constant  $\kappa$ . Here  $\{A, B\} = \sum_i \left( \frac{\partial A}{\partial q_i} \frac{\partial B}{\partial p_i} - \frac{\partial A}{\partial p_i} \frac{\partial B}{\partial q_i} \right)$  are the Poisson brackets.

The  $G_i(\mathbf{p}, \mathbf{q})$  ( $i = 1, \dots, R$ ) are  $R$  arbitrary phase-space functions, originally controlling the manner of the coupling to the bath as in Eq. (4). The noise is white and gaussian as before.

In fact, we do not need to go into the details of the derivation, because it will be shown in what follows that this equation is a *bona-fide* Langevin equation in that it leads to the canonical distribution at temperature  $T$ . The definition of Equation (5) is completed by specifying that it should be understood *in the Stratonovitch sense*: in a discretized form all phase-space functions in the right hand side have to be evaluated as an average of their values in the previous and the incremented time.

Indeed, one can adopt *Itô's convention* so the r.h.s. is evaluated in the previous time, and the equation now reads:

$$\dot{A} = \kappa \{A, H\} + \sum_j \{A, G_j\} (\xi_j(t) + \{G_j, H\}) + T \{G_j, \{G_j, A\}\} \quad (6)$$

Two particular cases are  $G_i = -q_i \forall i$ ;  $\kappa = 1$ , which yields (1,2), and  $G_i = p_i \forall i$ ;  $\kappa = 0$  which yields the *massless* version of (1). Note that in general the Poisson brackets between the  $G_i$  need not vanish, in which case the equations (5) cannot be taken through a canonical transformation to the form (1).

Let us now turn to the (Fokker-Planck) equation satisfied by the probability distribution  $P(\mathbf{q}, \mathbf{p}, t)$ . It is a simple exercise (see [3] or [4]) to obtain this directly from equation (5) or (6). The result is:

$$\frac{\partial P}{\partial t} + \kappa \{P, H\} = \sum_j \{G_j, \{G_j, H\} P + T \{G_j, P\}\} \quad (7)$$

It is now clear that  $P = \exp(-H/T)$  is a stationary solution of (7). Again, with the choice  $G_i = -q_i \forall i$ ;  $\kappa = 1$  we obtain the Kramer's equation. If instead we make  $G_i = p_i \forall i$ ;  $\kappa = 0$  we obtain the usual Fokker-Planck equation for diffusion without inertia.

By writing  $\langle A \rangle(t) = \int d\mathbf{q} d\mathbf{p} A(\mathbf{q}, \mathbf{p}) P(\mathbf{q}, \mathbf{p}, t)$  we obtain for the evolution of the average of an observable  $A(\mathbf{q}, \mathbf{p})$ :

$$\frac{d\langle A \rangle(t)}{dt} = \langle \{A, H\} \rangle - \sum_i \langle \{G_i, A\} \{G_i, H\} \rangle - T \sum_i \langle \{G_i, \{A, G_i\}\} \rangle \quad (8)$$

All three equations (5), (7) and (8) are canonically invariant in form: a canonical transformation of variables is obtained directly by transforming  $H$  and the  $G_i$ . Furthermore, the pure Hamiltonian term and the bath-coupling terms are explicitly separated.

### Equilibration

In order to study the equilibration properties, let us define an  $\mathcal{H}$ -function as [5] [6] :

$$\mathcal{H}(\sqcup) = \int [\mathbf{q} [\mathbf{p} \mathcal{P}(\mathbf{q}, \mathbf{p}, \sqcup) (\mathcal{T} \ln \mathcal{P}(\mathbf{q}, \mathbf{p}, \sqcup) + \mathcal{H}(\mathbf{q}, \mathbf{p}))] \quad (9)$$

which cannot increase, since:

$$\dot{\mathcal{H}}(t) = - \sum_i \int d\mathbf{q} d\mathbf{p} \frac{(\{G_i, H\} P + T \{G_i, P\})^2}{P} \leq 0 \quad (10)$$

Note that only the bath-terms contribute.

If the equilibrium measure exists,  $\mathcal{H}$  is bounded from below, and we have that

$$\{G_i, H\} P + T \{G_i, P\} \rightarrow 0 \quad \forall i \quad (11)$$

If we parametrize  $P(\mathbf{q}, \mathbf{p}, t)$  as:

$$P(\mathbf{q}, \mathbf{p}, t) = Q(\mathbf{q}, \mathbf{p}, t) \exp(-H/T) \quad (12)$$

the limit (11) implies that, once stationarity is achieved :

$$\{G_i, Q\} = 0 \quad \forall i \quad (13)$$

Using this equation, we have that  $\dot{Q} = \{H, Q\}$ . Since at stationarity (13) has to be valid at all times, we obtain the necessary conditions:

$$\{G_i, Q\} = 0 \quad ; \quad \{G_i, \{H, Q\}\} = 0 \quad ; \quad \{G_i, \{H, \{H, Q\}\}\} = 0 \quad ; \quad \dots \quad (14)$$

In the usual Langevin case (1,2),  $G_i = x_i$ ,  $H = \sum_i p_i^2/2m + V(x)$  and the first two sets of equations suffice to prove that  $Q = \text{constant}$  is the only stationary solution.

### Constants of Motion

Suppose the Hamiltonian has some constants of motion  $\{H, K_a\} = 0$ . Depending on the choice of  $G_i$ , these constants will be preserved or not by the coupling with the bath. Indeed, Eq. (5) implies:

$$\frac{dK_a}{dt} = \sum_j \{K_a, G_j\}(\xi_j(t) + \{G_j, H\}) \quad (15)$$

The evolution of  $K_a$  is then purely dictated by the heat-bath, and will be ‘slow’ in the small noise limit.

If we wish to construct a  $K_a$ -preserving noisy dynamics we have to choose the  $G_i$  such that  $\{K_a, G_i\} = 0 \forall i$ .

If, on the other hand, we couple the system to the bath through some constants of motion, that is  $G_i = K_i$ , the Langevin dynamics for any  $A(\mathbf{q}, \mathbf{p})$  becomes:

$$\dot{A} = \kappa \{A, H\} + \sum_j \{A, K_j\} \xi_j(t) \quad (16)$$

which expresses the fact that the system receives random kicks in the direction generated by the  $K_j$ .

An extreme and rather amusing form of this is the case in which we put a single  $G = H$  and  $\kappa = 0$ . We then have

$$\dot{A} = \{A, H\} \xi(t) \quad (17)$$

and the associated Fokker-Planck equation:

$$\frac{\partial P}{\partial t} = T \{H, \{H, P\}\} \quad (18)$$

The system diffuses back and forth along its classical trajectories. The probability distribution tends for long times to the smallest invariant structure compatible with the original distribution, and the entropy  $\int d\mathbf{q} d\mathbf{p} P(\mathbf{q}, \mathbf{p}, t) \ln P(\mathbf{q}, \mathbf{p}, t)$  becomes stationary.

### Motion within a Group

Another simple application is the construction of a heat-bath dynamics on a group. Suppose the Hamiltonian is constructed in terms of the generators  $L_i$  of a group, satisfying  $\{L_i, L_j\} = C_{ijl} L_l$ . Then,

$$\dot{L}_i = \{L_i, H\} + C_{ijl} L_l (\xi_j(t) + \{L_j, H\}) = C_{ijl} (\omega_j + \xi_j) L_l + C_{ijl} C_{jsr} \omega_s L_r L_l \quad (19)$$

where the ‘angular velocities’ are defined as  $\omega_i = \partial H(\mathbf{L}) / \partial L_i$ . The group invariant  $\sum_i L_i^2$  is clearly a constant of motion.

In summary, we have presented a manifestly canonical-invariant form of the langevin and Fokker-Planck equations. Within this formulation several questions originating from the underlying classical mechanics become more transparent.

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